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16. ABSTRACT

The occurrence of long range and interurban transport of ozone and/or ozone precursors across the Northeast U.S. has been documented by numerous field studies during the last ten years. The U.S. Environmental Protection Agency initiated the Northeast Corridor Regional Modeling Project (NECRMP) during the late 1970's, in part, to develop a regional model capable of simulating regional transport of ozone and its precursors on scales on the order of 1000 km. The resulting Regional Oxidant Model (ROM) is being applied to the Northeast U.S. to evaluate the effectiveness of various control strategies for reducing ozone in this region. This paper summarizes the physical processes encompassed by the model including several that have heretofore been omitted from air quality models on smaller scales, such as cumulus cloud effects on vertical atmospheric motions and nighttime wind shear. The general modeling framework that forms the basis of the ROM system of data preprocessors is also described. Model results from the first simulated episode of the NECRMP data base are presented.

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REGIONAL OXIDANT MODELING OF THE NORTHEAST U.S.

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INTRODUCTION

The development and application of a photochemical model capable of simulating regional transport of ozone and its precursors are the focus of an extensive program now in progress at the U.S. Environmental Protection Agency (EPA). This model, the Regional Oxidant Model (ROM) is designed for use in evaluating the effectiveness of various emission control strategies on a regional (1000 km) scale. The first model application will be for the Northeast U.S. where various studies have demonstrated the occurrence of widespread episodes of high ozone concentrations.[1,2] The purposes of this paper are to describe the basis and structure of the ROM including design and implementation considerations and to present some preliminary model results.

REGIONAL OXIDANT MODEL - THEORETICAL BASIS

The ROM has been designed to simulate most of the important chemical and physical processes responsible for the production of photochemically produced ozone on scales of 1000 km, or several days of transport time. These processes include horizontal transport, atmospheric chemistry, nighttime wind shear and turbulence episodes associated with the nocturnal jet, cumulus cloud effects on vertical mass transport and photochemical reaction rates, mesoscale vertical motions induced by terrain and the large scale flow, terrain effects on advection, diffusion and deposition, sub-grid scale chemistry processes, emissions of natural and anthropogenic precursors, and wet and dry removal processes. They are mathematically simulated in the 3-D Eulerian model with 3 1/2 vertical layers including the boundary layer and the capping inversion or cloud layer. Horizontal resolution varies slightly over the model domain because the ROM domain is defined in terms of curvilinear coordinates. For the first model application, horizontal resolution is approximately 18.5 km.

Vertical Structure

Detailed descriptions of the theoretical basis and design of the ROM

*On assignment from the National Oceanic and Atmospheric Administration, U.S. Department of Commerce.

are available elsewhere.[3,4] This section presents a brief summary of some of the unique features of the model. Figure 1 displays the vertical structure during daytime conditions. The top 3 layers are prognostic (predictive) and are free to locally expand and contract in response to changes in the physical processes occurring therein. During an entire simulation period horizontal advection and diffusion and gas phase chemistry are modeled prognostically in the upper 3 layers. The bottom layer is a shallow diagnostic surface layer designed to approximate the sub-grid scale effects on chemical reaction rates from a spatially heterogeneous emissions distribution.

During the day, the top model layer, layer 3, represents the synoptic-scale subsidence inversion, the base of which is typically 1-2 km above the ground. A downward flux of stratospheric ozone, specified as a boundary condition, may be considered in this layer. Also, if cumulus clouds are present, an upward flux of ozone and precursor species is injected into the layer by penetrative convection. At night, ozone and the remnants of other photochemical reaction products may remain in this layer and be transported long distances downwind. These processes are included in layer 3. Layers 1 and 2, above the surface layer, model the depth of the well-mixed layer during the day. In local areas where strong winds exist or the surface heat flux is weak there can exist substantial wind shear in the lowest few hundred meters above ground. This phenomenon can be treated separately in layer 1. Also, over large lakes or near seacoasts there often exists a thermal internal boundary layer that can be modeled in layer 1. Deposition on terrain features that protrude above the surface layer are also handled here. At night layer 2 represents the remains of the daytime mixed layer. As stable layers form near the ground and suppress turbulent vertical mixing a nocturnal jet forms above the stable surface layer and can transport aged pollutant products and reactants considerable distances. This jet is modeled in layer 1. Periodically the jet breaks down and allows sporadic episodes of vertical mixing at night between layer 1 and the surface layer, which is a reservoir of nighttime emissions from low level sources. At night, emissions from tall stacks and warm cities are injected directly into layers 1 and 2 aloft.

Surface Layer

The surface layer, model layer 0, parameterizes processes occurring within the lowest 100 m above ground. They include the sub-grid scale effects on chemical reaction rates from the spatially heterogeneous species concentrations resulting from point and line source emissions injections, the stagnation of surface emissions in stable surface layers, and the deposition of pollutants on vegetation and other surfaces. The variability of pollutant species concentrations within the ROM grid cells can have a significant effect on second-order chemical processes, such as occur in photochemical smog reactions. In averaging species concentrations over the volume of one grid cell information is lost concerning the fine scale structure. This may potentially cause erroneous reaction rates for NO, NO_2, and O_3 to be calculated. This problem can be made less severe by minimizing the averaging interval for rate calculations or parameterizing the fine structure effects. The latter approach is taken in the ROM.

In essence, layer 0 is simply a sophisticated lower boundary condition on layer 1. It is designed to estimate species concentrations in a diagnostic manner using current concentrations from layer 1 immediately above, along with local values of independent parameters such as emissions flux values and deposition velocities. An advantage of this design is that no additional computer storage is required beyond that needed for the other 3 model layers. Implicit in the design of layer 0 parameterization

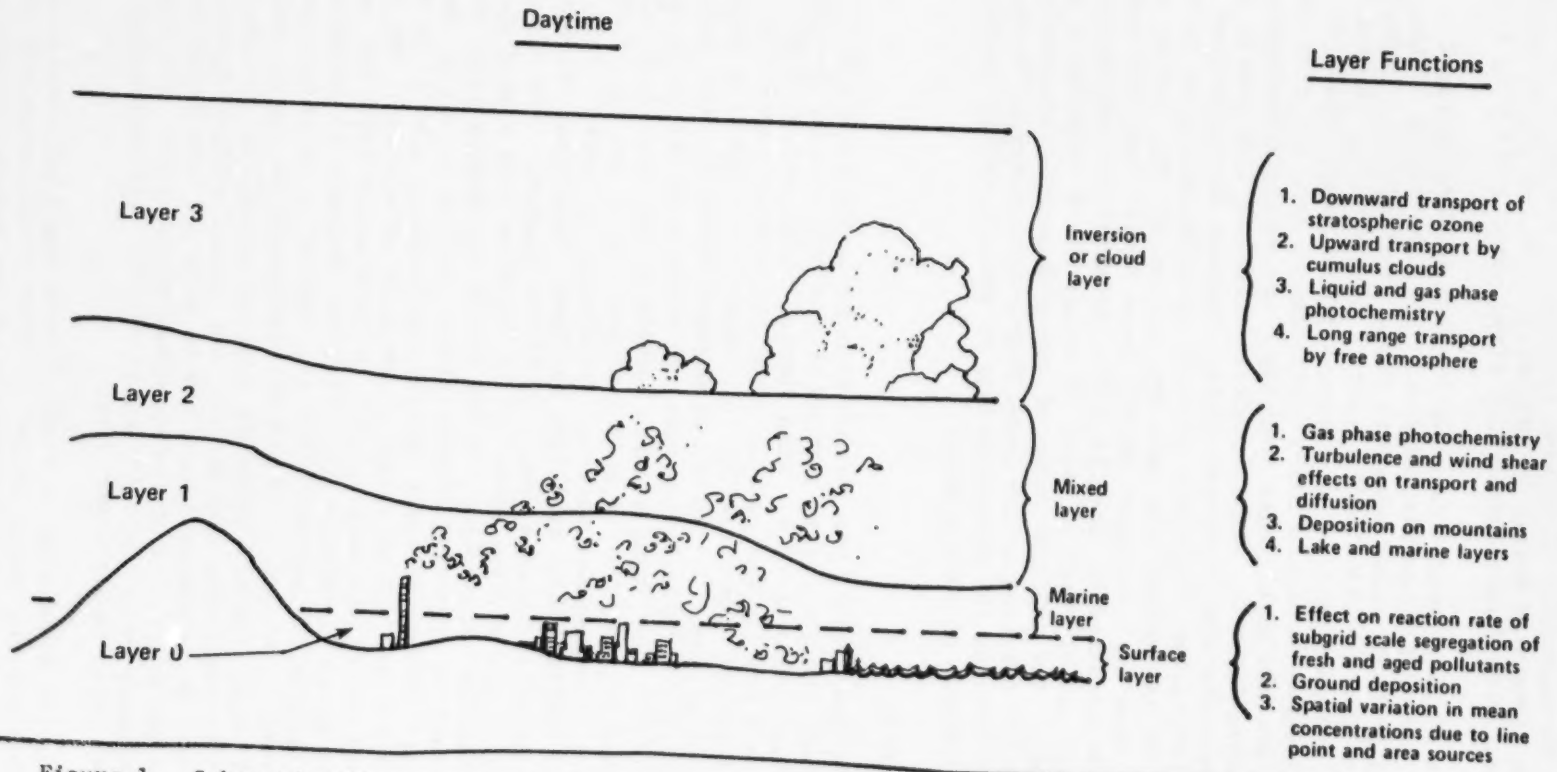
Daytime
Layer Functions
Layer 3
Layer 2
Layer 1
Layer 0
Inversion or cloud layer
Mixed layer
Marine layer
Surface layer
1. Downward transport of stratospheric ozone
2. Upward transport by cumulus clouds
3. Liquid and gas phase photochemistry
4. Long range transport by free atmosphere
1. Gas phase photochemistry
2. Turbulence and wind shear effects on transport and diffusion
3. Deposition on mountains
4. Lake and marine layers
1. Effect on reaction rate of subgrid scale segregation of fresh and aged pollutants
2. Ground deposition
3. Spatial variation in mean concentrations due to line point and area sources

Figure 1. Schematic illustration of the ROM vertical layer structure during the daytime.

is the assumption that horizontal transport within the layer is negligibly small and that the effects from phenomena occurring here are transferred to the rest of the model domain only through vertical mass fluxes. One of the benefits of the parameterization scheme is that it provides an estimate of the magnitude of spatial variations in layer 0 concentrations. This will be especially useful in comparing predicted cell-averaged concentrations with values observed at fixed point monitoring sites.

Outside of the plumes from emission line sources in layer 0, pollutant species are considered somewhat aged and thus, the ratios of their concentrations are probably close enough to their chemical equilibrium values (computed in layer 1) that little reaction occurs during the time that species are resident in layer 0. Thus, all pollutants except NO, NO_2, and O_3 are treated as pseudo-inert substances in that the time scales of their reactions are much larger than the characteristic residence time of material within layer 0. Within reactive emissions line source plumes chemical reactions should proceed rapidly because concentrations of NO_x are greatly disturbed from their chemical equilibrium values by fresh emissions. It is assumed that only the species NO, NO_2, and O_3 undergo significant chemical conversion within these plumes, and thus are the only species to be affected by sub-grid scale concentration variations within layer 0. The rate of reaction among these species is considered to be infinite here. The expected range of sub-grid scale concentrations is a function of the fraction of the layer 0 grid cell occupied by source emissions plumes and the concentrations of the particular species both inside and outside of such plumes.

Cloud Processes

As mentioned above, the effects from processes occurring in layer 0 propagate into the prognostic portion of the model domain through upward vertical fluxes into layer 1. When cumulus clouds are present in a layer 3 cell above a cell in the surface layer the vertical mass flux is partially diverted from injection into layer 1 to injection into the cumulus cloud of layer 3. In the atmosphere strong thermal vertical updrafts, primarily originating near the surface in the lowest portion of the mixed layer, feed young growing cumulus clouds with vertical air currents that extend from the ground to well above the top of the mixed layer in one steady upward motion. The dynamic effects of this transport process and daytime cloud evolution may have significant effects on the chemical fate of pollutants caught up in the process. For example, fresh emissions from the surface layer may be injected into a warm thermal and rise, essentially unperturbed, to the top of the mixing layer where they enter the base of a growing cumulus cloud. Within the cloud the chemical processes of ambient pollutant species are suddenly altered by the presence of liquid water and the attendant attenuation of sunlight. The presence of young cumulus clouds implies that the atmosphere above the earth's boundary layer is too stably stratified for thermals to penetrate higher. When this happens the air composing the tops of these clouds dives back into the mixed layer and is heated by compression on its descent. Eventually the liquid water droplets evaporate leaving behind the residue of the aqueous phase reactions. Ultimately, the parcel arrives again at the surface level where new emissions may be injected into it and ground deposition may occur, and the process may begin again. The time required for one complete cycle would typically be 30-50 min with perhaps one-tenth of the time spent in the cloud stage.

Within the ROM system, a sophisticated sub-model simulates this cloud flux process and its impact on the material fluxes among all the model's layers. In the current implementation of the chemical kinetics, liquid phase chemistry is not modeled and thus part of the effects from the

cloud flux processes are not accounted for in the simulations. Future versions of the chemical kinetics may include liquid phase reactions. The magnitude of the mass flux proceeding directly from the surface layer to the cloud layer is modeled as being proportional to the observed amount of cumulus cloud coverage and inversely proportional to the observed depth of the clouds.

Chemical Mechanism

Initial testing with the ROM has used a simplified chemical kinetic mechanism of gas phase photochemistry of the NO_x-HC-O_3 system developed by Demerjian.[5] This kinetics mechanism will be replaced with the latest available Carbon Bond chemical mechanism[6] before the final version of the model is complete. The newer chemical mechanism will be more detailed than the Demerjian mechanism and will include explicit reaction pathways for the naturally emitted organic species that have been included in the source emissions data base for the Northeast U.S. application. The current ROM version distributes the natural organic species among the existing lumped reactivity classes.

Horizontal Transport

Horizontal transport within the top 3 layers is governed by hourly wind fields interpolated from periodic wind observations made from upper air soundings and surface measurements. During the nighttime simulation period the lowest few hundred meters of the atmosphere above the ground may become stable as a radiation inversion forms near the ground. This entire layer is "decoupled" from the rest of the old daytime mixed layer. Wind speeds increase in this inversion layer and the nocturnal jet forms, capable of carrying ozone, other reaction products, and emissions from tall stacks and warm cities considerable distances downwind. This phenomenon is potentially quite significant in modeling regional scale air quality and is parameterized in the ROM layer 1.

In classical studies of short-range dispersion, atmospheric motion is assumed to consist of 2 distinct components: a large-scale, uniform flow and small-scale fluctuations in the flow, or turbulence. The premise that these components are universal characteristics of atmospheric flow supports the common practice in air pollution models of representing the mean flow by a mathematical expression fit to hourly averaged wind observations and parameterizing the turbulence effects by eddy diffusivities whose values are taken from empirical data. Lamb[3] shows how these assumptions are not necessarily a sound basis for representing atmospheric motion in regional dispersion models. He then develops a conceptual and mathematical basis for representing fluid motion that is consistent with classical definitions of transport and turbulence of short-range boundary layer diffusion and also with dispersion over arbitrarily large scales. Within this conceptual framework is the notion that a uniquely correct flow field can not be determined from a discrete set of wind observations on the regional scale. In fact when one attempts to fit a continuous field to such data using some objective analysis technique, one finds that each technique produces a somewhat different field. The constraints imposed by the various techniques are simply mathematical procedures that are not necessarily relevant to the physics of the system. Away from areas near wind observations it is very difficult to choose the best representation from among the various interpolations.

A technique is developed to derive a discrete set or family of possible flow fields that is consistent with both the observations and the physical laws governing the system. Each flow realization, given a fixed emissions source distribution, maps onto a resultant concentration

field after model simulation. It is impossible to predict which concentration field would occur at any one time from among the full set of resultant fields. From this predicted set of concentrations and an estimate of their probability of occurrence, one can specify the frequency with which the actual concentration can be expected to fall within a given interval of values in a large number of observations. The width of this interval is a measure of the "predictability" of the concentration estimate. This approach to air quality modeling is a break from the traditional manner of using models in an absolute fashion and it is a much more realistic approach for the regional scale.

REGIONAL OXIDANT MODEL - STRUCTURE AND ORGANIZATION

The key components of the modeling system are illustrated in Figure 2. The system requires six types of "raw" data inputs: air quality, meteorology, emissions, cloud cover, land use, and topography. These "raw" data inputs are manipulated by a network of processors which range in function from simple reformatting of emissions data to generating the complex families of wind fields which drive the atmospheric transport. The functions of the principal processors are summarized in Table I. These processors are interconnected by their requirements for and production of data. The ultimate product of the processor network is a collection of data files which can be categorized into two types: processor input files (PIF) and model input files (MIF). Processor input files contain partially processed data required as input to higher level processors. Model input files also provide input to a number of high level processors, however they primarily contain the parameter fields which are transformed into matrix elements and variables required by the model algorithms.

The processors are organized into six distinct hierarchical levels. Level 1 processors interface directly with the "raw" input data sets. These "raw" data sets have, in fact, undergone extensive quality control. Processors at any level can interface directly with the B-Matrix compiler (BMC) described below, by production of model input files. This multi-level organization is important to the network because it clearly delineates the sequence of program execution. Processors at the same level may execute simultaneously. However, a processor at any given level must wait until all processors along its lower level input data paths have been completed. Formal definition of all data/processor relationships and automation of processor executions are essential to ensure consistency and validity of model input files.

The program which serves as the interface between the model input files and the algorithms describing the governing processes is called the B-Matrix Compiler (BMC) because it functions similar to a computer language compiler which transforms high level language commands into a machine/algorithm specific representation. The BMC mathematically combines physical parameters such as wind components, horizontal eddy diffusivities, etc. into the complex coefficients required for solution of the governing equations. These coefficients can no longer be equated with physical reality; they are purely mathematical entities related specifically to the form of the generalized finite difference algorithms used by the ROM.

The core of the ROM system is a set of algorithms which solve the coupled set of generalized finite difference equations that describe the governing processes in each layer of the model. These governing equations have been expressed in a form which allows the chemical kinetics, advection and vertical flux to be treated independently. The chemistry module exchanges information with algorithms of the governing equations via two vectors. One vector contains the net production rate of each species and

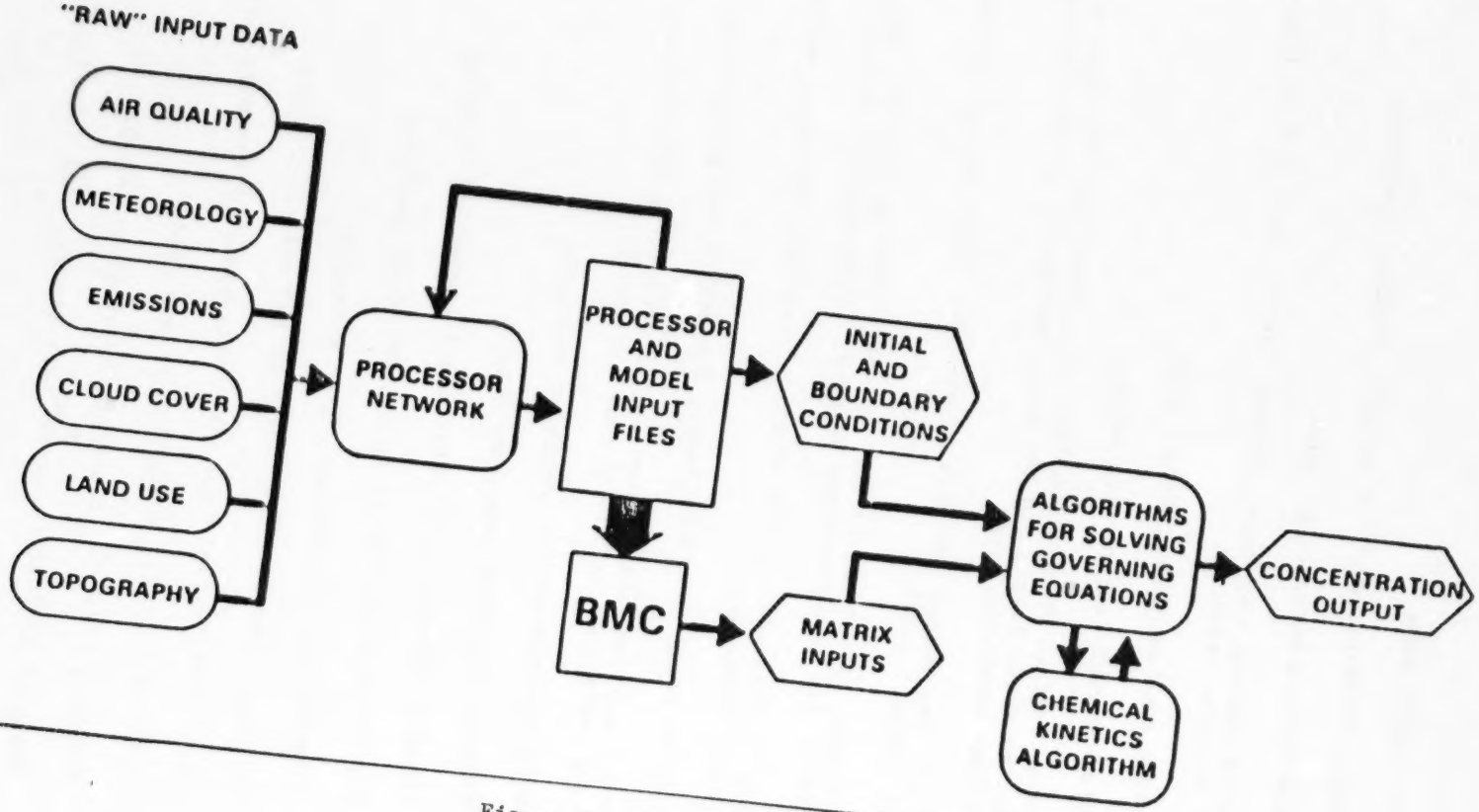

Figure 2. ROM system overview.

Table I. Processor Function Summary

Processor Name	Function
P01	Prepares rawind data
P02	Determines initial, upper and lateral boundary conditions
P03	Prepares surface meteorology data
P04	Estimates surface roughness, Obukhov length, surface heat flux and friction velocity
P05	Processes cumulus cloud fraction data
P06	Computes averaged terrain elevations
P07	Computes terrain penetration fractions, simulates the depth of the daytime shear layer, and the depth and motion of the nighttime surface inversion layer
P08	Computes parameters specifying pollutant fluxes across top surfaces of layers 2 and 3.
P09	Calculates adjustment factors for variation of chemical rate constants due to atmospheric density, temperature, and cloud cover
P10	Computes emissions source strength functions and plume volume fraction parameter
P11	Computes families of vertically integrated horizontal winds
P12	Computes parameters to describe interfacial material fluxes, and estimates horizontal eddy diffusivities
P13	Estimates line source length in each grid
P14	Prepares emissions inventory data
P15	Computes deposition resistance and deposition velocity
P16	Interpolates rawinds to hourly upper air profiles
P17	Computes time derivatives of cell heights
P19	Computes fractional sky coverage for all cloud types
P21	Classifies initial condition concentrations for each cell
P25	Prepares land use fractions in each grid
P28	Computes B-Matrix parameters required by the ROM
P29	Computes diffusivities and back tracked cell locations

the other vector contains the net destruction rate of each species. Such design simplifications enhance the flexibility of the model and have been extended to allow interchange not only of the chemistry mechanism, but of all theoretical formulations of the physical and meteorological processes, i.e., the processors.

Thus the structure of the ROM system provides a flexible modeling framework with both permanent and interchangeable components. The permanent components are:

- o the algorithmic form of the governing equations
- o the B-Matrix Compiler
- o the processor and model input files
- o the data interfaces between components and processors

The formal design specification for the ROM system intentionally separates functional components from "fixed" data interfaces. This modular structure provides several benefits:

- o ability to easily modify process descriptions and chemical kinetics mechanism
- o ability to modify the general framework to handle other regional scale problems - visibility, particulate, acid deposition
- o support of structured design techniques and team implementation
- o simplification of testing, debugging and error isolation

Once such a general modeling framework is operational, continuous upgrading to state-of-the-art methodologies is not only feasible, but also practical. The long term usefulness of this framework for atmospheric modeling research and applications tremendously outweights any additional efforts required to develop flexibility in the framework rather than a specific model. Ultimately, the difference in effort is primarily in the design, not in the implementation.

APPLICATION TO NECRMP/NEROS DATA BASE

The NECRMP ambient data base was assimilated from field data collected during EPA measurement programs conducted in 1979 and 1980 in the northeastern U.S. Figure 3 shows the horizontal extent of the ROM domain as applied to this data base. The NECRMP data base consists of measurements of 4 field experiments: the 1979 Northeast Regional Oxidant Study (NEROS I), the 1980 NEROS II, the Persistent Elevated Pollution Episodes Study (PEPE), and the 1980 Urban Field Studies. Together, these studies have provided a variety of air quality and meteorological measurements on regional, urban and site-specific scales.[7]

Upper air meteorological sounding data were available from 10 National Weather Service (NWS) stations located within the model domain and from 14 additional sites surrounding the region and extending into Canada that are required to resolve boundary conditions. The frequency of balloon releases at selected NWS sites was increased during the EPA field measurement programs from the usual 2 per day at 12 hour intervals to 4 per day at 6 hour intervals. In addition, the NECRMP data base consists

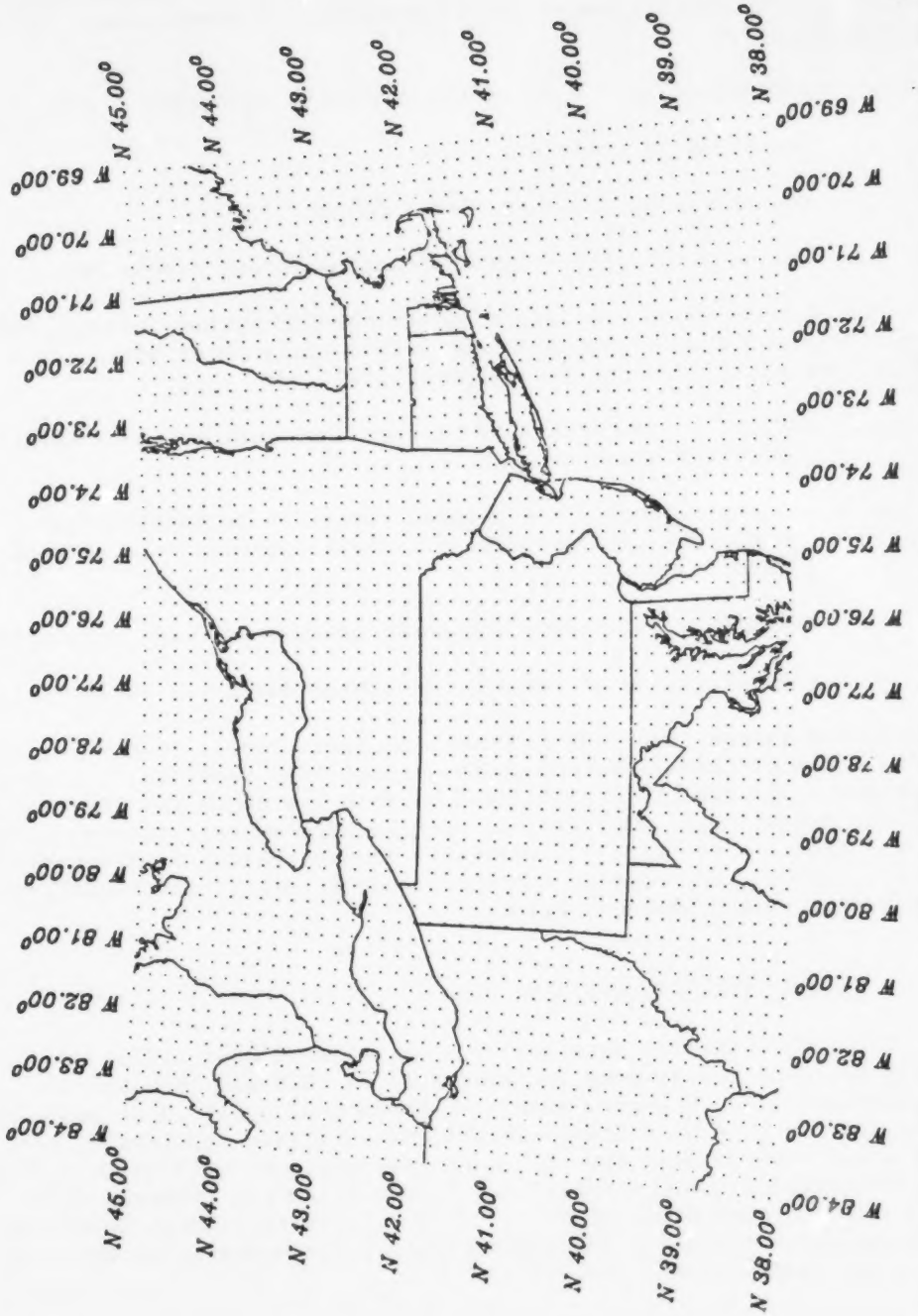

Figure 3. Modeling region and grid resolution in the ROM application.

of upper air data from 12 special supplementary sites for radiosonde and pibal releases and 4 sodar locations aligned from Virginia to Massachusetts. Also, meteorological data from tetroons, small and large tethered balloons and minisondes are available. The hourly surface meteorological data base consists of data from 160 NWS stations in the U.S. and Canada, 41 special NECRMP sites and 27 State and local monitoring sites.

Aircraft were also used to collect meteorological and air quality data during the NECRMP field studies. The flight patterns designed during the 1979 field studies were set up to provide horizontal and vertical distributions of measured parameters within specific air parcels as they were transported across the region. The 1980 field study flights included designs to characterize urban plumes, examine urban plume interactions, and also to characterize the regional air mass pollutant concentrations. Among the parameters measured by the aircraft were O_3, NO, NO_x, SO_2, b-scat, temperature, relative humidity, and periodic canister samples for hydrocarbon species analysis. Surface air quality data were collected at 81 State and local sites scattered across the modeling region and 79 special NECRMP sites aligned along the East coast urban corridor.

The EPA, in conjunction with the individual states in the ROM modeling domain, compiled a complete 1979/1980 NECRMP emissions inventory[8] specifically addressing the ROM requirements. Environment Canada provided emissions information for those portions of Canada included in the domain. Major point sources, or those stationary sources typically emitting greater than 100 tons per year of any pollutant, are classified separately from mobile and small stationary sources. For electric utilities, state-specific seasonal allocation factors are calculated from power generation statistics and hourly factors are derived from hourly power plant fuel use data. Other point source categories rely on plant-specific operating data for temporal resolution of emissions. Annual area source emissions are temporally subdivided based on information gathered from the literature and previous studies. County emissions are apportioned to the modeling grid system based on the known distribution of surrogate indicators such as housing, population, urban land, agricultural land, composite forestland, airport and port locations.

The individual grid cells composing the ROM grid for the NECRMP application shown in Figure 3 are 15 minutes of longitude wide in the E-W direction and 10 minutes of latitude in the N-S direction, or about 18.5 km square cells. There are 60 cells E-W and 42 cells N-S. Several multi-day periods from the data base will be chosen for model simulation.

Initial testing with the first generation (preliminary) ROM has focused on the period of August 3-5, 1979 during the NECRMP/NEROS I project. Episodic air stagnation conditions occurred over the central and western portions of the region covered by the ROM domain during this period. Rain and showers terminated the elevated pollutant concentration levels along the immediate East Coast. Figure 4 shows the predicted O_3 concentration pattern for model layer 1 using one of the possible wind fields generated from the observed data for the period. These concentrations are valid for 1600h (LST) on August 4. The primary O_3 plume, with concentrations in excess of 0.25 ppm, is shown over Lake Ontario, having drifted to the northeast from the Cleveland-Buffalo vicinity earlier in the simulation. A second area of high concentrations, between 0.12 and 0.16 ppm is shown downwind of the Detroit-Windsor area. The plumes shown along the East Coast are probably overestimated in the model predictions because the ROM does not include the physical and chemical effects of precipitation events. The location and magnitude of the primary O_3 plume generally correspond to that shown by aircraft data analyzed from the NEROS I project.[9] The aircraft sampled the air mass in a Lagrangian

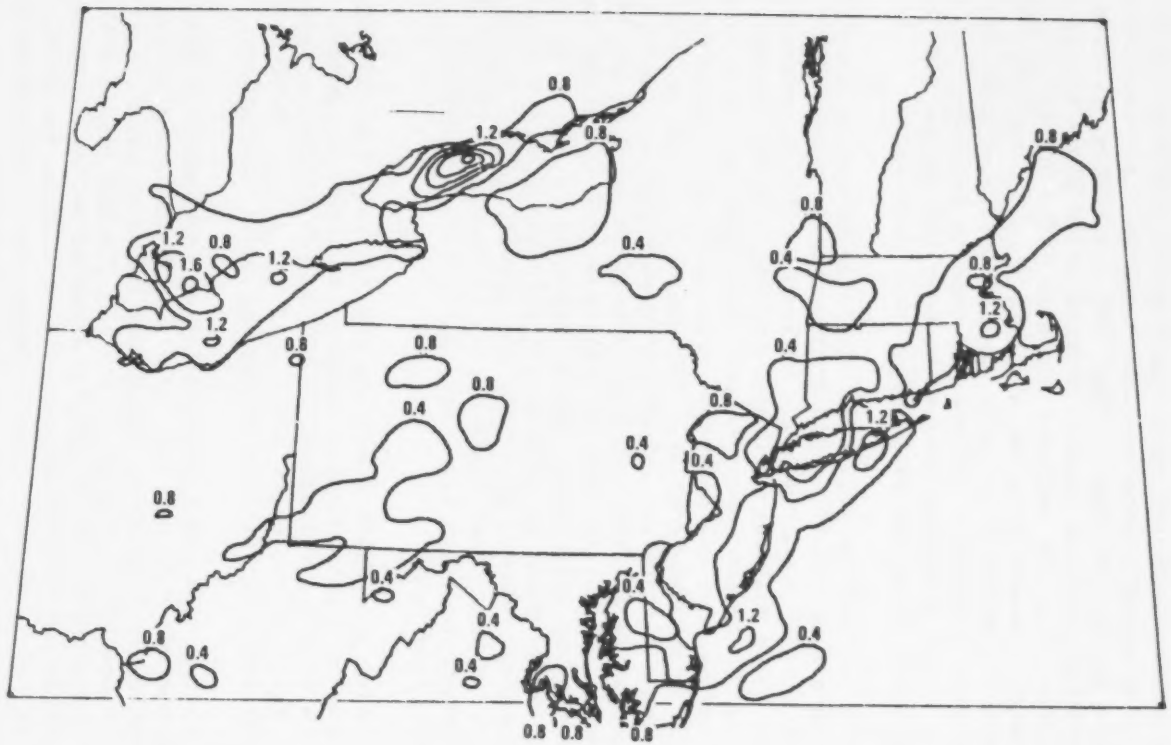

Figure 4. Contours of predicted O_3 values (in ppm x 10) from the ROM for Aug. 4, 1979 for the NEROS region.

fashion and had measured concentrations the previous evening in the area south of Buffalo at levels up to 0.130 ppm in the remains of the mixed layer. A quantitative model evaluation study will be performed with the ROM and the NECRMP/NEROS data base in the near future. While testing is now being done using the 1979 portion of the data base, the evaluation study will be based on the independent 1980 data set.

SUMMARY

EPA's Regional Oxidant Model was designed to simulate the physical and chemical processes that are responsible for photochemical smog within the earth's boundary layer on a 1000 km horizontal scale. This tool thereby provides a means for understanding the regional transport phenomenon and aids in planning for effective control strategies to mitigate the ozone pollutant burden. The framework for the model includes 3 prognostic layers in the vertical extending through to the top levels of cumulus cloud convection and a shallow diagnostic surface layer designed to account for the sub-grid scale chemical effects of a heterogeneous emissions distribution. Among the processes accounted for are advective transport, photochemistry, nighttime wind shear and turbulence episodes, cumulus cloud effects on vertical mass transport and photochemical reaction rates, terrain influences, biogenic and anthropogenic emissions, and removal by deposition. The uncertainties in defining a regional scale flow field from a limited set of observations are quantified by defining a finite set of wind field "realizations" that are all consistent with the observations and with underlying physical principles. Air quality predictions at specific sites resulting from model simulations with this set of wind fields would take the form of expected probability distributions.

The ROM was designed in a modular fashion that provides for a flexible modeling framework with both permanent and interchangeable components. The interchangeable components include the chemical kinetics mechanism and the model preprocessors that can be periodically updated to include state-of-the-art formulations.

The initial data base for regional model application is that collected during the NECRMP field studies of 1979-80 in the Northeast U.S. For this application the model domain has 60 grid cells E-W and 42 cells N-S with a grid spacing of approximately 18.5 km. Several multi-day periods from the data base will be chosen for model simulation. Results from initial tests qualitatively show major O_3 plumes to be in agreement with field project observations.

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